

Section 9

SOLID-STATE PHYSICS

H. P. R. FREDERIKSE, Editor

The National Bureau of Standards

CONTENTS

| | |
|---|-------|
| 9a. Crystallographic Properties..... | 9-2 |
| 9b. Structure, Melting Point, Density, and Energy Gap of Simple Inorganic Compounds..... | 9-10 |
| 9c. Electronic Properties of Solids..... | 9-26 |
| 9d. Properties of Metals..... | 9-38 |
| 9e. Properties of Semiconductors..... | 9-56 |
| 9f. Properties of Ionic Crystals..... | 9-74 |
| 9g. Properties of Superconductors..... | 9-127 |
| 9h. Color Centers and Dislocations..... | 9-148 |
| 9i. Luminescence..... | 9-158 |
| 9j. Work Function and Secondary Emission..... | 9-172 |

9a. Crystallographic Properties

J. D. H. DONNAY¹

The Johns Hopkins University

W. P. MASON AND E. A. WOOD²

Bell Telephone Laboratories, Inc.

9a-1. Crystal System, Space Group, Cell Content, Lattice Constants, Structure Type. These data are presented for all the chemical elements (Table 9a-2) and for certain selected compounds (Table 9a-3).

In each table the first column contains the *chemical formula*, with mention of the polymorphic form, if necessary, and of the temperature, if known, at which the lattice constants have been determined.

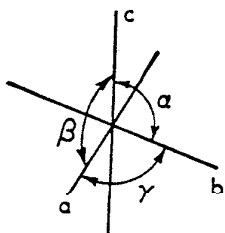


FIG. 9a-1. Coordinate axes (= "crystallographic axes").

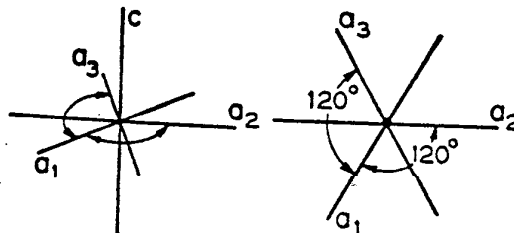


FIG. 9a-2. Coordinate axes for the hexagonal system (can also be used for the rhombohedral system).

The *crystal system*, listed in column 2, is based on the point symmetry of the lattice³ of the crystal structure. It is given by the initial letter of its name (see Table 9a-1). The coordinate axes x, y, z are taken along three concurrent cell edges that form a right-handed system (a, b, c in Fig. 9a-1; a_1, a_2, c in Fig. 9a-2). Symmetry governs the relative values of the unit lengths a, b, c and of the interaxial angles α, β, γ . The symmetry requirements entail a specialization of the lattice constants (Table 9a-1) and a corresponding reduction in the number of values that must be listed in the tables of data.

The *space group* is given (Tables 9a-2 and 9a-3, column 3) in both Schoenflies and Hermann-Mauguin notations. The symbols of the 32 crystal point groups, needed for comparison with the space-group symbols, will be found in Table 9a-1, where the

¹ Crystallographic Data.

² Tensor Properties of Crystals.

³ "Lattice" *s.s.*: triperiodic assemblage of points, the termini of the vectors $L(uvw) = ua + vb + wc$, where u, v, w take all integral values—the geometrical expression of a translation group, described by a repeating parallelepiped ("cell") whose edges are preferably chosen along symmetry axes of the lattice.

Hermann-Mauguin symbol is given for every orientation and the Schoenflies symbol follows between parentheses.

A Hermann-Mauguin *point-group symbol* states what symmetry a specified discontinuous vectorial property possesses along certain directions of the crystal. These directions are those of the symmetry axes of the lattice (Table 9a-1, column 2). They are grouped in sets of equivalent directions, some being chosen as cell edges as shown in Table 9a-1 (column 3). An Arabic numeral represents a rotation axis of symmetry along one direction (*examples*: any 2 in 222 , the 3 in $3m$) or along each direction of a set (the 2 in $\bar{4}2m$, either 2 in 622 , the 3 in $m\bar{3}m$). Surmounted by a bar the numeral indicates a rotatory-inversion axis. *Example*: the $\bar{4}$ axis stands for a cyclic group in which the first power of the symmetry operation is a 90 deg rotation followed by an inversion through a point¹ on the axis—the fixed point in the point group. The $\bar{1}$ axis

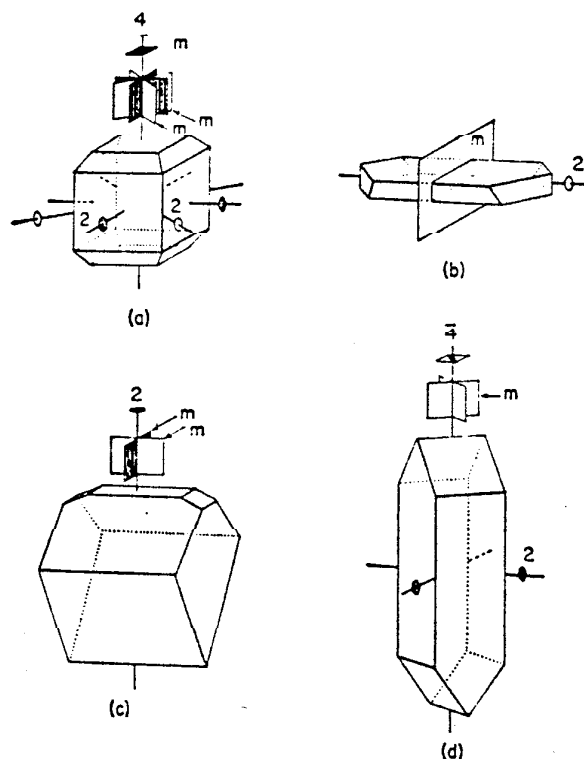


FIG. 9a-3. Examples of macroscopic crystal symmetry (point groups): (a) tetragonal, $4/mmm$; (b) monoclinic, $2/m$; (c) orthorhombic, mm ; (d) tetragonal, $\bar{4}2m$. (After W. P. Mason and E. A. Wood.)

is not defined in direction: it symbolizes the center of symmetry. A mirror plane of symmetry, designated m , is perpendicular to the direction it describes. *Example*: in $6/mmm$ the first m is perpendicular to the c axis, the second m and the third m represent three mirrors each that are perpendicular to a_1 , a_2 , a_3 and the bisectors, respectively. The following point groups contain the center of symmetry: mmm ($= 2/m\ 2/m\ 2/m$), $m\bar{3}m$ ($= 4/m\ \bar{3}\ 2/m$), $m\bar{3}$ ($= 2/m\ \bar{3}$), $\bar{3}$, and N/m , where N is an even number. Figure 9a-3 illustrates the assemblages of symmetry elements in four selected point groups, which express the morphological symmetry of well-formed crystals.

A Hermann-Mauguin *space-group symbol* begins with a capital letter that tells the lattice mode: primitive (P), body-centered (I), one-face-centered (C , A , or B), all-face-centered (F), rhombohedral (R). Additional symmetry elements appear. In a

¹ Note that this point is *not* a center of symmetry.

TABLE 9a-1. THE SEVEN CRYSTAL SYSTEMS BASED ON THE POINT SYMMETRY OF THE LATTICE

| Name | Lattice symmetry (holohedry) | Symmetry directions ^a | Restrictions imposed by symmetry | Tabulated values | Merohedries (subgroups of the lattice symmetry in each system ^e) |
|----------------------------------|------------------------------|---|--|----------------------------------|--|
| Anorthic..... (= triclinic) | $I(C_1)$ | None | None | $a, b, c, \alpha, \beta, \gamma$ | $I(C_1)$; |
| Monoclinic..... | $2/m(C_{2h})$ | b | $\gamma = \alpha = 90^\circ$ $\alpha = \beta = \gamma = 90^\circ$ | a, b, c, β a, b, c | $m(C_2), 2(C_2)$ $mm2[2mm](C_{2v}), 222(D_2)^\dagger$; |
| Orthorhombic..... (= rhombic) | $mmm(D_{2h})$ | $(c)(ab)$ (bisectors) ^c | $b = a, \alpha = \beta = \gamma = 90^\circ$ | a, c | $42m\bar{4}m2(D_{2d}), 4mm(C_{4h}), 422(D_4)$; $4/m(C_{4h}), \bar{4}(S_4), 4(C_2)$; |
| Tetragonal..... | $4/mmm(D_{4h})$ | $(c)(a_1a_2a_3)$ (bisecc.) ^c | $b = a, \alpha = \beta = 90^\circ, \gamma = 120^\circ$ | a, c | $\{5m\bar{2}52m(D_{5h}), 6mm(C_{6h}), 622(D_6)\}$; $6/m(C_{6h}), \bar{6}(C_{6h}), 6(C_2)$; |
| Hexagonal..... | $6/mmm(D_{6h})$ | $(c)(a_1a_2a_3)$ | $b = a, \alpha = \beta = 90^\circ, \gamma = 120^\circ$ | a, c | $3m[31m](D_{3d}), 3m\bar{1}[31m](C_{3h}), 321[312](D_3)$; $3(C_2), 3(C_3)^\ddagger$; |
| Rhombohedral ^b | $3m(D_{3d})$ | (abc) (b.d.) ^d | $b = c = a, \alpha = \beta = \gamma = \alpha$ $b = c = a, \alpha = \beta = \gamma = 90^\circ$ | a, a, α a | $3m(C_{3v}), 32(D_3)$; $3(C_2), 3(C_3)^\ddagger$; $43m(T_d), 432(O)$; $m\bar{3}(T_h), 23(T)$ |
| Cubic..... (= isometric) | $m\bar{3}m(O_h)$ | (abc) (b.d.) (f.d.) ^d | | | |

^a Symmetry directions in the lattice (in the same sequence as in the Hermann-Mauguin symbol), and how cell edges are chosen from them.
^b A rhombohedral lattice can be described by means of a triple cell, which has the same shape as the cell of a hexagonal lattice (a, c) but has additional points at $\frac{1}{2}$ | and $\frac{1}{2}$ | (fractions of a_1, a_2, c , respectively), or by means of the primitive rhombohedral cell (a_1, a_2, a_3). Both descriptions are given in Tables 9a-2 and 9a-3.
^c Bisectors of the angles between the axes: a_1b, a_2b, a_3b and a_1a_2, a_2a_3, a_3a_1 .
^d The four body diagonals (b.d.) and the six face diagonals (f.d.) of the cube.
^e Semicolons separate the 11 Laue classes.
^f Alternate orientations, shown between brackets, are needed in space-group symbols.
^g All five trigonal point groups appear in both hexagonal (H) and rhombohedral (R) systems.

TABLE 9a-2. CRYSTALLOGRAPHIC DATA FOR THE ELEMENTS

| Formula (temp., °C, for the lattice constants given) | Crystal system | Space group ^a | Z | Lattice constants, ^b a, b, c; α, β, γ | Structure type |
|---|-------------------|--------------------------|--------|---|-----------------------|
| Ar (extrapolated, 0K) | Cub. | O_h^h-Fm3m | 4 | 5.3109 ± 0.0001 | A1 (f.c.c.) |
| Ag (25) | Cub. | O_h^h-Fm3m | 4 | 4.08641 Å* | A1 (f.c.c.) |
| Al (24.8) | Cub. | O_h^h-Fm3m | 4 | 4.04964 | A1 (f.c.c.) |
| As (26) | Rhdr. | $D_{3d}^5-R\bar{3}m$ | 6 | 3.700, 10.548 | A7 |
| | | | 2 | (a_r 4.132, α 54°07½') | |
| Au (25) | Cub. | O_h^h-Fm3m | 4 | 4.0786 | A1 (f.c.c.) |
| B | Tetr. | $D_{2d}^{10}-P4_2/nm$ | 50 | 8.74, 5.07 | |
| Ba (26) | Cub. | O_h^h-Im3m | 2 | 5.025 | A2 (b.c.c.) |
| Be (18) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 2.2854, 3.5807 | A3 (h.c.p.) |
| Be (630)(stable 500-700) | Hex. | | ca. 60 | 7.1, 10.8 | |
| Bi (25) | Rhdr. | D_{3d}^5-R3m | 6 | 4.546, 11.860 | A7 (As) |
| | | | 2 | (a_r 4.745, α 57°14½') | |
| Br ₂ (-150) | Orth. | $D_{2h}^{12}-Bmab$ | 4 | 6.68, 8.74, 4.49 | A14 (I ₂) |
| C (diamond)(26) | Cub. | O_h^h-Fd3m | 8 | 3.5667 | A4 (diamond) |
| C (graphite)(14.6) | Hex. | $D_{6h}^4-P6_3/mmc$ | 4 | 2.4612 ± 0.0001, 6.7079 ± 0.0007 | A9 |
| C (graphite) | Rhdr. | D_{3d}^5-R3m | 6 | 2.461, 10.064 | |
| | | | 2 | (a_r 3.842, α 39.49°) | |
| Ca (α)(electrolytic) | Cub. | O_h^h-Fm3m | 4 | 5.582 ± 0.004 | A1 (f.c.c.) |
| Ca (γ)(above 464) | Cub. | O_h^h-Im3m | 2 | 4.477 ± 0.007 | A2 (b.c.c.) |
| Cd (26) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 2.9793, 5.6181 | A3 (h.c.p.) |
| Ce (γ) | Cub. | O_h^h-Fm3m | 4 | 5.150 ± 0.002 | A1 (f.c.c.) |
| Ce (β) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.66, 5.97 | A3 (h.c.p.) |
| Ce (α) | Cub. | O_h^h-Fm3m | 4 | 5.1612 ± 0.0005 | A1 (f.c.c.) |
| Ce (δ)(stable above 730) | Cub. | O_h^h-Im3m | 2 | 4.11 | A2 (b.c.c.) |
| Cl ₂ (-185) | Tetr. | $D_{2d}^{10}-P4_2/nm$ | 8 | 8.58, 6.13 | A18 |
| Co (α)(20) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 2.5074, 4.0699 | A3 (h.c.p.) |
| Co (20) | Cub. | O_h^h-Fm3m | 4 | 3.5442 | A1 (f.c.c.) |
| Cr | Cub. | T_d^2-I43m | 58 | 8.735 | A12 (αMn) |
| Cr (25) | Cub. | O_h^h-Im3m | 2 | 2.8845 ± 0.0005 | A2 (b.c.c.) |
| Cs (-100) | Cub. | O_h^h-Im3m | 2 | 6.09 | A2 (b.c.c.) |
| Cu (25) | Cub. | O_h^h-Fm3m | 4 | 3.61509 ± 0.00004 | A1 (f.c.c.) |
| Dy (99.8% pure) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.5903 ± 0.0001, 5.6475 ± 0.0002 | A3 (h.c.p.) |
| Er (99.8% pure) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.5588 ± 0.0003, 5.5874 ± 0.0003 | A3 (h.c.p.) |
| Eu (98-99% pure) | Cub. | O_h^h-Im3m | 2 | 4.606 ± 0.001 | A2 (b.c.c.) |
| Fe (α)(20)(stable to 900) | Cub. | O_h^h-Im3m | 2 | 2.86645 ± 0.00001 | A2 (b.c.c.) |
| Fe (γ)(stable 900-1400) | Cub. | O_h^h-Fm3m | 4 | 3.64 | A1 (f.c.c.) |
| Fe (δ)(stable above 1400) | Cub. | O_h^h-Im3m | 2 | 2.94 | A2 (b.c.c.) |
| Ga (unstable form)(-16.3) | Orth. | D_{2h}^4-Amam | 4 | 3.17, 8.13, 2.90, all ± 0.03 | |
| Ga (stable form) | Orth. | $D_{2h}^{15}-Abam$ | 8 | 4.524, 7.661, 4.523 | A11 |
| Gd (99.7% pure) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.6360 ± 0.0009, 5.7826 ± 0.0006 | A3 (h.c.p.) |
| Ge (24.6) | Cub. | O_h^h-Fd3m | 8 | 5.657764 ± 0.000010 Å* | A4 (diamond) |
| H ₂ (above 1.30 K) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.761 ± 0.007, 6.105 ± 0.011 | A3 (h.c.p.) |
| He ⁺ (3.48 K, 163 atm) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.501, 5.721 | A3 (h.c.p.) |
| He ⁺ (3.95 K, 129 atm) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.470, 5.540 | A3 (h.c.p.) |
| Hf (26) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.1967, 5.0578 | A3 (h.c.p.) |
| Hg (5 K) | Rhdr. | $D_{3d}^5-R\bar{3}m$ | 3 | 3.457, 6.664 | A10 |
| | | | 1 | (a_r 2.9863, α 70° 44.6') | |
| Ho (99.4% pure) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.5773 ± 0.0001, 5.6158 ± 0.0002 | A3 (h.c.p.) |
| I ₂ (26 ± 1) | Orth. | $D_{2h}^{12}-Bmab$ | 4 | 7.271, 9.803, 4.792 | A14 |
| In (26) | Tetr. | $D_{3d}^{17}-I4/mmm$ | 2 | 3.2517, 4.9459 | A6 |
| Ir (26) | Cub. | O_h^h-Fm3m | 4 | 3.8394 | A1 (f.c.c.) |
| K (20) | Cub. | O_h^h-Im3m | 2 | 5.344 ± 0.005 | A2 (b.c.c.) |
| Kr (-252.5) | Cub. | O_h^h-Fm3m | 4 | 5.60 | A1 (f.c.c.) |
| Kr (89 K) | Cub. | O_h^h-Fm3m | 4 | 5.709 ± 0.014 | A1 (f.c.c.) |
| La (α)(99.8% pure) | Hex. | | 4 | 3.770 ± 0.002, 12.159 ± 0.003 | |
| La (β)(stable above ca. 260) | Cub. | O_h^h-Fm3m | 4 | .307 ± 0.002 (99.6% pure) | A1 (f.c.c.) |
| La (γ)(stable above 864 C) | Cub. | O_h^h-Im3m | 2 | 4.26 | A2 (b.c.c.) |
| Li ⁺ (20) | Cub. | O_h^h-Im3m | 2 | 3.5092 ± 0.0006 | A2 (b.c.c.) |
| Li ⁺ (20) | Cub. | O_h^h-Im3m | 2 | 3.5107 ± 0.0009 | A2 (b.c.c.) |
| Li (-195) | Cub. | O_h^h-Im3m | 2 | 3.491 ± 0.002 | A2 (b.c.c.) |
| Li (-195) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.111 ± 0.001, 5.093 ± 0.009 | A3 (h.c.p.) |
| Li (-195) | Cub. | O_h^h-Fm3m | 4 | 4.404 ± 0.030 (induced by deformation) | A1 (f.c.c.) |
| Lu (99.9% pure) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.5031 ± 0.0004, 5.5509 ± 0.0004 | A3 (h.c.p.) |
| Mg (25°)(99.995% pure) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.20939 ± 0.00003, 5.21053 ± 0.00005 Å* | A3 (h.c.p.) |

TABLE 9a-2. CRYSTALLOGRAPHIC DATA FOR THE ELEMENTS (Continued)

| Formula (temp., °C. for the lattice constants given) | Crystal system | Space group ^a | Z | Lattice constants, ^b a, b, c; α , β , γ | Structure type |
|---|-------------------|---|-----|---|-------------------|
| Mn (α) | Cub. | $T_d^2-I\bar{4}3m$ | 58 | 8.911 \pm 2 | A12 (type) |
| Mn (β) (stable 705-1100) | Cub. | $O_h^2-Fm\bar{3}c$ | 160 | 12.61 | A13 (type) |
| Mn (γ) | Tetr. | $D_{6h}^{17}-I4/mmm$ | 2 | 2.671 \pm 0.002, 3.533 \pm 2 | |
| Mo (25) | Cub. | $O_h^2-Fm\bar{3}m$ | 2 | 3.1472 | A2 (b.c.c.) |
| Mo | Cub. | $O_h^2-Fm\bar{3}m$ | 4 | 4.16 (precipitated in vacuo) | A1 (f.c.c.) |
| N ₂ (α) (20 K) (stable below 35.6 K) | Cub. | $T_h^2-Pa\bar{3}$ | 4 | 5.661 \pm 0.008 | |
| N ₂ (β) (50 K) (stable 35.6-63.1 K) | Hex. | $P6_3/mmc$ | 2 | 3.93 \pm 0.16, 6.50 \pm 51 | |
| Na | Cub. | $O_h^2-Fm\bar{3}m$ | 2 | 4.2906 \pm 0.0005 | A2 (b.c.c.) |
| Na (-195) | Cub. | $O_h^2-Fm\bar{3}m$ | 4 | 5.350 (induced by deformation at -253°) | A1 (f.c.c.) |
| Nb (20) (H ₂ -free) | Cub. | $O_h^2-Fm\bar{3}m$ | 2 | 3.3008 \pm 0.0003 | A2 (b.c.c.) |
| Nd (α) (99.8% pure) | Hex. | | 4 | 3.6579 \pm 0.0003, 11.7992 \pm 0.0005 | |
| Nd (β) (stable above 862) | Cub. | $O_h^2-Fm\bar{3}m$ | 2 | 4.13 | A2 (b.c.c.) |
| Ne (3 K) | Cub. | $O_h^2-Fm\bar{3}m$ | 4 | 4.446 \pm 0.009 | A1 (f.c.c.) |
| Ni (25) (99.99% pure) | Cub. | $O_h^2-Fm\bar{3}m$ | 4 | 3.52394 \pm 0.00008 | A1 (f.c.c.) |
| O ₂ (α) (stable below 23.5 K) | | | | | |
| O ₂ (β) (stable 23.5-43.4 K) | | | | | |
| O ₂ (γ) (50 K) | Cub. | $O_h^2-Pm\bar{3}n$ | 8 | 6.83 \pm 0.05 | |
| O ₈ (26) | Hex. | $D_{6h}^{17}-P6_3/mmc$ | 2 | 2.7341, 4.3197 | A3 (h.c.p.) |
| P ₄ (white) (-30) | Cub. | $T_d^2-I\bar{4}3m$, or $O_h^2-I\bar{4}3!$ | 56 | 18.51 \pm 0.03 | |
| P (black) (22) | Orth. | $D_{2h}^{12}-Abam$ | 8 | 4.3763 \pm 0.0005, 10.478 \pm 0.001, 3.3136 \pm 0.0005 | A17 |
| P (red) | Mon. | | | 7.34 (pseudocubic), 11.31 (cubic) | |
| Pb (25) (99.999% pure) | Cub. | $O_h^2-Fm\bar{3}m$ | 4 | 4.9505 | A1 (f.c.c.) |
| Pd (25) | Cub. | $O_h^2-Fm\bar{3}m$ | 4 | 3.9898 | A1 (f.c.c.) |
| Po (α) (10 \pm 10) ^d | Cub. | $O_h^2-Pm\bar{3}m$ | | 3.345 \pm 0.002 | |
| Po (β) (75 \pm 15) ^d | Rhdr. | $D_{3d}^5-R\bar{3}m$ | | 2.222, 2.151 | |
| Pr (α) (99.9% pure) | Hex. | | 4 | (a_1 3.359 \pm 0.002, 98° 13' \pm 3') | |
| Pr (β) | Cub. | $O_h^2-Fm\bar{3}m$ | 4 | 3.6725 \pm 0.0007, 11.8354 \pm 0.0012 | A1 (f.c.c.) |
| Pt (25) | Cub. | $O_h^2-Fm\bar{3}m$ | 4 | 5.161 \pm 0.002 | A1 (f.c.c.) |
| Pu (α) (21) (stable 122 \pm 2) | Mon. | $C_{2h}^2-P2_1/m$ | 16 | 3.9231 | A1 (f.c.c.) |
| Pu (β) (190) (stable to 206 \pm 3) | Mon. | C_{2h}^2-I2/m | 34 | 10.973 \pm 0.001, 4.8244 \pm 0.0005, 6.1835 \pm 0.0005, 101.81° | |
| Pu (γ) (235) ^d (stable to 319 \pm 5) | Orth. | D_{2h}^2-Fddd | 8 | 0.284, 10.403, 7.809, 92.13° \pm 0.03° 5.7682 \pm 0.0004, 10.162 \pm 0.002, 3.1587 \pm 0.0004 | |
| Pu (δ) (320) (stable to 451 \pm 4) | Cub. | $O_h^2-Fm\bar{3}m$ | 4 | 4.6370 | A1 (f.c.c.) |
| Pu (ϵ) (477) (stable to 476 \pm 5) | Tetr. | $D_{6h}^{17}-I4/mmm$ | 2 | 3.339 \pm 0.003, 4.446 \pm 0.007 | |
| Pu (ζ) (490) (liquid at 610 \pm 2) | Cub. | $O_h^2-Fm\bar{3}m$ | 2 | 3.6361 \pm 4 (99.97% pure) | A2 (b.c.c.) |
| Rb (19) | Cub. | $O_h^2-Fm\bar{3}m$ | 2 | 5.709 | A2 (b.c.c.) |
| Re (20) | Hex. | $D_{6h}^{17}-P6_3/mmc$ | 2 | 2.7608 \pm 0.0004, 4.4582 \pm 0.0003 | A3 (h.c.p.) |
| Rh (18) | Cub. | $O_h^2-Fm\bar{3}m$ | 4 | 3.8043 \pm 3 | A1 (f.c.c.) |
| Ru (20) | Hex. | $D_{6h}^{17}-P6_3/mmc$ | 2 | 2.70389, 4.28168 | A3 (h.c.p.) |
| S (β) (103) | Mon. | $C_{2h}^2-P2_1/c$ | 48 | 11.04, 10.98, 10.92, 96° 44' | |
| S (γ) | Mon. | C_{2h}^2-P2/n | 32 | 8.54, 13.08, 8.25, 112° 53' | |
| S ₈ (α) (24.8) | Orth. | D_{2h}^2-Fddd | 16 | 12.86654 \pm 0.00010, 24.48694 \pm 0.00026, 10.46500 \pm 0.00009 Å° | |
| S (unstable) | Rhdr. | $C_{2h}^2-R\bar{3}$ | 18 | 10.9, 4.27; a_1 6.46, α 115° 18' | |
| Sb (26) | Rhdr. | $D_{3d}^5-R\bar{3}m$ | 6 | 4.307, 11.273 | A7 |
| Sc (99.6% pure) | Hex. | $D_{6h}^{17}-P6_3/mmc$ | 2 | (a_1 4.506, α 57° 06') | A3 (h.c.p.) |
| Sc | Cub. | $O_h^2-Fm\bar{3}m$ | 2 | 3.3090 \pm 0.0001, 5.2733 \pm 0.0016 | A1 (f.c.c.) |
| Se (26) | Hex. | $D_{2h}^2-P3_121$ or $D_3^2-P3_121$ | 4 | 4.541 \pm 5 | A8 (type) |
| Se (α) | Mon. | $C_{2h}^2-P2_1/n$ | 32 | 11.61, 9.07, 9.05, \pm 0.01 90° 46' \pm 5' | |
| Se (β) | Mon. | $C_{2h}^2-P2_1/a$ | 32 | 12.85, 8.07, 9.31, \pm 0.01, 93° 08' \pm 5' | |
| Si (25) | Cub. | $O_h^2-Fd\bar{3}m$ | 8 | 5.43072 \pm 0.00005 | A4 (diamond) |
| Si (dense form) | Cub. | $T_d^2-Ia\bar{3}$ | 16 | 6.64 \pm 0.01 | |
| Sm | Rhdr. | $D_{3d}^5-R\bar{3}m$ | 9 | 3.829 \pm 0.002, 26.20 \pm 0.01 | |
| Sn (α , gray) (25) | Cub. | $O_h^2-Fd\bar{3}m$ | 3 | (a_1 8.982, α 23.31°) | A4 (diamond) |
| Sn (β , white) (25) | Tetr. | $D_{6h}^{17}-I4_1/amd$ | 4 | 6.489 (stable to 13.2°) 5.8318 \pm 0.0003, 3.1819 \pm .0003 | A5 |

TABLE 9a-2. CRYSTALLOGRAPHIC DATA FOR THE ELEMENTS (Continued)

| Formula (temp., °C. for the lattice constants given) | Crystal system | Space group ^a | Z | Lattice constants, ^b a, b, c; α , β , γ | Structure type |
|---|-------------------|---|----|---|-------------------|
| Sr (α)(25)(stable below 215 \pm 10) | Cub. | $O_h^h-Fm\bar{3}m$ | 4 | 6.0849 \pm 0.0005 | A1 (f.c.c.) |
| Sr (β)(248°)(stable 215-605) | Hex. | $D_{6h}^h-P6_3/mmc$ | 2 | 4.32 \pm 0.01, 7.06 \pm 0.01 | A3 (h.c.p.) |
| Sr (γ)(614°)(stable above 605 + 10) | Cub. | $O_h^h-I\bar{m}3m$ | 2 | 4.85 \pm 0.01 | A2 (b.c.c.) |
| Ta (25) | Cub. | $O_h^h-I\bar{m}3m$ | 2 | 3.3058 | A2 (b.c.c.) |
| Tb (99.9% pure) | Hex. | $D_{6h}^h-P6_3/mmc$ | 2 | 3.6010 \pm 0.0003, 5.6936 \pm 0.0002 | A3 (h.c.p.) |
| Tc | Hex. | $D_{6h}^h-P6_3/mmc$ | 2 | 2.741 \pm 0.001, 4.397 \pm 0.001 | A3 (h.c.p.) |
| Te (25) | Hex. | $D_{2h}^h-P3_121$ or $D_{3h}^h-P3_121$ | 3 | 4.4570, 5.9290 | A8 (Se) |
| Th (α)(stable below 1400)(25) | Cub. | $O_h^h-Fm\bar{3}m$ | 4 | 5.0847 \pm 0.0002 | A1 (f.c.c.) |
| Th (β)(1450) ^d | Cub. | $O_h^h-I\bar{m}3m$ | 2 | 4.11 \pm 0.01 | A2 (b.c.c.) |
| Ti (α)(25) | Hex. | $D_{6h}^h-P6_3/mmc$ | 2 | 2.950, 4.686 | A3 (h.c.p.) |
| Ti (β)(900°)(stable above 882 \pm 20) | Cub. | $O_h^h-I\bar{m}3m$ | 2 | 3.33 | A2 (b.c.c.) |
| Tl (α)(18)(99.995% pure) | Hex. | $D_{6h}^h-P6_3/mmc$ | 2 | 3.4496 \pm 0.0002, 5.5137 \pm 0.0004 | A3 (h.c.p.) |
| Tl (β)(262)(stable above 230) | Cub. | $O_h^h-I\bar{m}3m$ | 2 | 3.882 \pm 0.001 (99.995% pure) | A2 (b.c.c.) |
| Tm (99.9% pure) | Hex. | $D_{6h}^h-P6_3/mmc$ | 2 | 3.5375 \pm 0.0001, 5.55146 \pm 0.0004 | A3 (h.c.p.) |
| U (α)(24.6) | Orth. | $D_{2h}^h-I\bar{1}mam$ | 4 | 4.95572 \pm 0.00006, 5.87007 \pm 0.00006, 2.85373 \pm 0.00005 Å [*] | A20 |
| U (β)(stable 660-760) | Tetr. | $C_{4v}^h-P4_2nm$ or $D_{2d}^h-P4_2n2$ | 30 | 10.52, 5.57 | |
| U (γ)(stable, 760 to mp)(room temp.) | Cub. | $O_h^h-I\bar{m}3m$ | 2 | 3.474 \pm 0.005 | A2 (b.c.c.) |
| U (δ)(800) | Cub. | $O_h^h-I\bar{m}3m$ | 2 | 3.49 | A2 (b.c.c.) |
| V (25) | Cub. | $O_h^h-I\bar{m}3m$ | 2 | 3.0399 \pm 0.0003 | A2 (b.c.c.) |
| W (α)(25) | Cub. | $O_h^h-I\bar{m}3m$ | 2 | 3.16517 Å [*] | A2 (b.c.c.) |
| W (β) ^e (transforms irreversibly to α above 700) | Cub. | $O_h^h-Pm\bar{3}n$ | 8 | 5.048 \pm 0.003 | A15 |
| Xe (75.0 K \pm 0.5) | Cub. | $O_h^h-Fm\bar{3}m$ | 4 | 6.2023 \pm 0.0010 | A1 (f.c.c.) |
| Y | Hex. | $D_{6h}^h-P6_3/mmc$ | 2 | 3.6515 \pm 0.0002, 5.7474 \pm 0.0004 | A3 (h.c.p.) |
| Yb (99.9% pure) | Cub. | $O_h^h-Fm\bar{3}m$ | 4 | 5.4862 \pm 0.0004 | A1 (f.c.c.) |
| Zn (17) | Hex. | $D_{6h}^h-P6_3/mmc$ | 2 | 2.6589, 4.9349 | A3 (h.c.p.) |
| Zr (α)(25) | Hex. | $D_{6h}^h-P6_3/mmc$ | 2 | 3.232, 5.147 | A3 (h.c.p.) |
| Zr (β)(stable above 870)(979) | Cub. | $O_h^h-I\bar{m}3m$ | 2 | 3.616 \pm 0.002 | A2 (b.c.c.) |

^a Schoenflies symbol followed by Hermann-Mauguin symbol.

^b For nearly all the substances listed, the unit of length is the Å based on the 1948 values of the X-ray wavelengths [Acta Cryst. 1, 48 (1948)]. Pre-1949 values were published in kX units (1 kX = 1,000 X, where X is the unit used by Siegbahn to express his numerical values of X-ray wavelengths); they have been converted to Å by means of the relation 1 kX = 1.00202 Å. For highly accurate determinations, the original values have been converted to Bearden's redefined angstrom unit (1964), which is identified by an asterisk (Å^{*}); in the formula 1 kX = Λ Å^{*} the conversion factor Λ is the ratio λ_B/λ_S of the numerical values used by Bearden and Siegbahn for the wavelength of the X-ray line employed: Λ is equal to 1.002,061 for NiK α_1 ; 1.002,058 for CuK α_1 ; etc. Neither the Å nor the Å^{*} is a metric unit. The Å used in the tables is equal to 10⁻¹⁰ m within 1 in 25,000; the Å^{*}, within a few ppm. See J. W. M. Dumond, Proc. Natl. Acad. Sci. 45, 1052 (1959); J. A. Bearden, "X-ray Wavelengths," U.S. Atomic Energy Commission, Oak Ridge, Tenn., 1964.

^c H. E. Swanson et al., NBS Monograph 25(4), p. 3, 1966.

^d W. B. Pearson, "A Handbook of Lattice Spacings and Structures of Metals and Alloys," Pergamon Press, New York, 1958-1967.

^e For controversy on the existence of W(β), see R. L. Moss and I. Woodward, Acta Cryst. 12, 255 (1959).

screw axis the numeral carries a subscript (example, 6₂); this means that the rotation is accompanied by a glide parallel to the axis and equal to a fraction of the corresponding lattice translation (in 6₂ the glide that accompanies a rotation of 360 deg/6 amounts to 3/6 of c). In a *glide plane* the reflection is combined with a glide parallel to the plane and equal to half a lattice translation; the glide plane is designated by a letter that identifies this lattice translation as being: a cell edge (a, b, or c),¹ the diagonal of the unit parallelogram (*mesh*) of the net in the plane (n), or half the diagonal if the mesh is centered (d). To read the point-group symmetry of a crystal from its space-group symbol: skip the capital letter, replace every small letter by m, and omit all subscripts (example: P2₁/a gives 2/m).

¹ In R3c and R3c the c is that of the hexagonal description (a,c).

TABLE 9a-3. CRYSTALLOGRAPHIC DATA FOR SELECTED COMPOUNDS

| Formula (temp., °C, for the lattice constants given) | Crystal system | Space group ^a | Z | Lattice constants, ^b a, b, c; α , β , γ | Structure type |
|--|-------------------|--|----|--|---------------------------|
| AgCl (26) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 5.5491 | B_1 (NaCl) |
| AgBr (26) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 5.7745 | B_1 (NaCl) |
| Al ₂ O ₃ (α) (corundum) (24.7) | Rhdr. | $D_{3d}^2-R\bar{3}c$ | 6 | 4.759216 \pm 0.000027, 12.99127 \pm 0.00024 (a_r 5.12863; 55°17.36') | D51 |
| Al ₂ O ₃ (β) | Hex. | $D_{6h}^4-P6_3/mmc$ | 12 | 5.57, 22.60 | D56 |
| BaTiO ₃ | Tetr. | D_{4h}^2-P4/mmm | 1 | 3.9939, 4.0346 | Deformed G5 |
| BaTiO ₃ (200) | Cub. | $O_h^3-Fm\bar{3}m$ | 1 | 4.0121 \pm 0.0005 | G5 |
| CaCO ₃ (calcite) (18) | Rhdr. | $D_{3d}^2-R\bar{3}c$ | 6 | 4.9898 \pm 0.0003, 17.060 \pm 0.005 (a_r 6.3748; 46°04.8') | G1 |
| CaCO ₃ (aragonite) | Orth. | $D_{2h}^{12}-Pnam$ | 4 | 5.741, 7.968, 4.959 | G2 (type) |
| CaF ₂ (fluorite) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 5.46398 \pm 0.00007 Å [*] | C1 (type) |
| CdI ₂ (type 2H) (25) | Hex. | $D_{3h}^2-P\bar{3}m1$ | 1 | 4.24, 6.835 | C6 |
| CoFe ₂ O ₄ | Cub. | $O_h^3-Fd\bar{3}m$ | 8 | 8.429 \pm 0.005 | H11 (spinel) ^c |
| COOK·(CHOH) ₂ ·COONa·4H ₂ O (Rochelle salt) | Orth. | $D_{2h}^2-P2_12_12$ | 4 | 11.93, 14.33, 6.18 | |
| CsBr (α) (25) | Cub. | $O_h^3-Fm\bar{3}m$ | 1 | 4.2953 | B2 (CsCl) |
| CsD ₃ (β) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 7.23 \pm 0.02 | B1 (NaCl) |
| CaCl (25) | Cub. | $O_h^3-Fm\bar{3}m$ | 1 | 4.10 \pm 0.02 | B2 (type) |
| CaCl (β) (500) (stable above 460) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 7.09 \pm 0.02 | B1 (NaCl) |
| CsI (α) (26) | Cub. | $O_h^3-Fm\bar{3}m$ | 1 | 4.5679 | B2 (CsCl) |
| CsI (β) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 7.66 \pm 0.02 | B1 (NaCl) |
| Fe ₃ O ₄ (26) (iron ferrite or magnetite) | Cub. | $O_h^3-Fd\bar{3}m$ | 8 | 8.396 | H11 (spinel) ^c |
| KBr (25 \pm 0.2) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 6.5982 \pm 0.0002 | B1 (NaCl) |
| KCl (25) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 6.29294 \pm 0.00008 | B1 (NaCl) |
| KF (20) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 5.347 | B1 (NaCl) |
| KI (25) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 7.06555 \pm 0.00015 | B1 (NaCl) |
| LiBr (26) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 5.5013 | B1 (NaCl) |
| LiCl (25) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 5.13988 \pm 0.00004 | B1 (NaCl) |
| LiF (25 \pm 0.2) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 4.0262 \pm 0.0001 | B1 (NaCl) |
| KH ₂ PO ₄ (26) | Tetr. | $D_{2d}^{12}-I\bar{4}2d$ | 4 | 7.448, 6.977 | H22 |
| MgAl ₂ O ₄ (spinel) | Cub. | $O_h^3-Fd\bar{3}m$ | 8 | 8.0800 | H11 (type) |
| MgFe ₂ O ₄ | Cub. | $O_h^3-Fd\bar{3}m$ | 8 | 8.359 \pm 0.005 | H11 (spinel) ^c |
| MgO (25) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 4.213 | B1 (NaCl) |
| MnFe ₂ O ₄ (20) | Cub. | $O_h^3-Fd\bar{3}m$ | 8 | 8.499 | H11 (spinel) ^c |
| NaBr (25) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 5.9737 | B1 (NaCl) |
| NaBrO ₃ | Cub. | T^2-P2_13 | 4 | 6.72 | G3 |
| NaCl (26) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 5.6402; also reported; 5.64009 \pm 0.00003 (25°) | B1 (type) |
| NaClO ₃ | Cub. | T^2-P2_13 | 4 | 6.568 \pm 0.001 | G3 |
| NaF (25) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 4.6342 | B1 (NaCl) |
| NH ₄ Br (250) (stable above 137.5) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 6.91 | B1 (NaCl) |
| NH ₄ Br (18) (stable below 137.5) | Cub. | $O_h^3-Fm\bar{3}m$ | 1 | 4.059 | B2 (CsCl) |
| NH ₄ Br (γ) (-100) | Tetr. | $D_{2d}^{12}-F\bar{4}d2$ | 1 | 4.257, 4.043, \pm 0.004 | B25 |
| NH ₄ Cl (250) (stable above 154.3) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 6.547 | B1 (NaCl) |
| NH ₄ Cl (26) (stable below 184.3) | Cub. | $O_h^3-Fm\bar{3}m$ | 1 | 3.9756 | B2 (CsCl) |
| NiAs (pure) | Hex. | $D_{6h}^4-P6_3/mmc$ | 2 | 3.638, 5.059 | B8 |
| NiFe ₂ O ₄ (25) | Cub. | $O_h^3-Fd\bar{3}m$ | 8 | 8.330 | H11 (spinel) ^c |
| NH ₄ H ₂ PO ₄ | Tetr. | $D_{2d}^{12}-I\bar{4}2d$ | 4 | 7.499, 7.548 | H22 |
| RbF | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 5.84 \pm 0.02 | B1 (NaCl) |
| RbF (~12 kb) | Cub. | $O_h^3-Fm\bar{3}m$ | 1 | 3.29 | B2 (CsCl) |
| RbCl (α) (-190) | Cub. | $O_h^3-Fm\bar{3}m$ | 1 | 3.749 | B2 (CsCl) |
| RbCl (β) (20) | Cub. | $O_h^3-Fm\bar{3}m$ | 4 | 6.548; also 6.5810 (27°) | B1 (NaCl) |
| TlCl (26) | Cub. | $O_h^3-Fm\bar{3}m$ | 1 | 3.8421 | B2 (CsCl) |
| TlBr (25) | Cub. | $O_h^3-Fm\bar{3}m$ | 1 | 3.9850 | B2 (CsCl) |
| TlI | Cub. | $O_h^3-Fm\bar{3}m$ | 1 | 4.208 | B2 (CsCl) |
| TlI (25) | Orth. | $D_{2h}^{12}-Amam$ | 4 | 5.251, 12.92, 4.582 | B33 |
| SiC (α) (type 2H) | Hex. | $C_{6v}^3-P6_3/mc$ | 2 | 3.076 \pm 0.001, 5.048 \pm 0.001 | (many types) |
| SiC (β) (25) | Cub. | $T_d^2-P\bar{4}3m$ | 4 | 4.3597 | B3 (ZnS) |
| SiO ₂ (low quartz stable up to 573 \pm 1) (25) | Hex. | $D_{3h}^2-P3_121$ or $D_{3h}^2-P3_221$ | 3 | 4.91343 \pm 0.00001, 5.40506 \pm 0.00003 Å [*] | C8, α |
| SiO ₂ (high quartz) (stable 573-870) | Hex. | $D_{6h}^4-P6_3/mmc$ or $D_{6h}^4-P6_422$ | 3 | 5.01, 5.47 | C8, β |
| SiO ₂ (high tridymite) (stable 570-1470) | Hex. | $D_{6h}^4-P6_3/mmc$ | 4 | 5.04, .24 (determined outside stability range?) | C10 |

TABLE 9a-3. CRYSTALLOGRAPHIC DATA FOR SELECTED COMPOUNDS (Continued)

| Formula (temp., °C. for the lattice constants given) | Crystal system | Space group ^a | Z | Lattice constants, ^b a, b, c; α , β , γ | Structure type |
|---|-------------------|--|-----|---|----------------------------------|
| SiO ₂ (low tridymite)..... | Hex. | | 864 | 30.08, 49.08 | |
| SiO ₂ (high cristobalite (stable 1470- 1710)..... | Cub. | T _h ^h -P2 ₃ | 8 | 7.1473 (at 1300°) | |
| SiO ₂ (coesite) (high pressure)..... | Mon. | C _{2h} ^h -C ₂ /c | 10 | 7.17, 12.38, 7.17, 120° | |
| ZnO (18)..... | Hex. | C _{6v} ^h -P6 ₃ mc | 2 | 3.2427 ± 0.0001, 5.1948 ± 0.0003 | B ₄ H ₀ |
| ZrSiO ₄ (zircon)..... | Tetr. | D _{2h} ¹² -I ₄ /amd | 4 | 6.58, 5.93 | |
| ZnS (sphalerite, blende) (contains 0.16 wt % Fe)..... | Cub. | T _d ^h -F ₄ 3m | 4 | 5.423 ± 0.006 | B ₃ |
| ZnS (wurtzite) (type 2H)..... | Hex. | C _{6v} ^h -P6 ₃ mc | 2 | 3.8231, 6.2613 | B ₄ |

^a Schoenflies symbol followed by Hermann-Mauguin symbol.

^b For nearly all the substances listed, the unit of length is the Å based on the 1948 values of the X-ray wavelengths. Acta Cryst. 1, 48 (1948). Pre-1949 values were published in kX units (1 kX = 1,000 X, where X is the unit used by Siegbahn to express his numerical values of X-ray wavelengths); they have been converted to Å by means of the relation 1 kX = 1.00202 Å. For highly accurate determinations, the original values have been converted to Bearden's redefined angstrom unit (1964), which is identified by an asterisk (Å*); in the formula 1 kX = λ Å* the conversion factor λ is the ratio λ_B/λ_S of the numerical values used by Bearden and Siegbahn for the wavelength of the X-ray line employed: λ is equal to 1.002,061 for NiK α_1 ; 1.002,058 for CuK α_1 ; etc. Neither the Å nor the Å* is a metric unit. The Å used in the tables is equal to 10⁻¹⁰ m within 1 in 25,000; the Å*, within a few ppm. See J. W. M. Dumond, Proc. Natl. Acad. Sci. 45, 1052 (1959); J. A. Bearden, "X-ray Wavelengths," U.S. Atomic Energy Commission, Oak Ridge, Tenn., 1964.

* "Spinel" and "inverse spinel" both belong to type H11.

The value of Z (Tables 9a-2 and 9a-3, column 4) is the number of formula units in the cell, the formula being expressed as in column 1, and the cell as in column 5.

The cell given in column 5 is chosen according to the conventions of the second edition of "Crystal data" (ref. 1). The numerical values have been updated from the manuscript of the forthcoming third edition. The substances known to crystallize in any given space group are listed in ref. 2.

The symbols in column 6 identify structure types in *Strukturbericht* (refs. 4 and 5): A1, cubic close packed (= face-centered cubic, f.c.c.); A2, body-centered cubic (b.c.c.); A3, hexagonal close packed (h.c.p.); A4, diamond-type structures; etc. In many cases the prototype of the structure is added between parentheses: A7(As), A8(Se), etc.

Illustrative References

1. Donnay, J. D. H., Gabrielle Donnay, E. G. Cox, Olga Kennard, and M. V. King: Crystal Data, Determinative Tables, 2d ed., *Am. Cryst. Assoc. Monograph 5*, Polycrystal Book Service, Box 11567, Pittsburgh, Pa., 1963.
2. Nowacki, W.: Crystal Data, Systematic Tables, 2d ed., *Am. Cryst. Assoc. Monograph 6*, Polycrystal Book Service, Pittsburgh, Pa., 1967.
3. Palache, C., H. Berman, and C. Frondel: "The System of Mineralogy," 7th ed., vols. 1-3, John Wiley & Sons, Inc., New York; Chapman & Hall, Ltd., London, 1944, 1951, 1962.
4. Strunz, H.: "Mineralogische Tabellen," 5th ed., Akademische Verlagsgesellschaft Geest & Portig K.-G., Leipzig, 1969.
5. "Structure Reports," the continuation of "Strukturbericht," published for the International Union of Crystallography by N. V. A. Oosthoek's, Utrecht, Netherlands. "Strukturbericht," a digest of crystal-structure literature from 1913 through 1939, published in conjunction with *Z. Krist.*
6. Wyckoff, R. W. G.: "Crystal Structures," 2d ed., vols. 1-5, Interscience Publishers, a division of John Wiley & Sons, Inc., New York, 1963-1966.
7. Pearson, W. B.: "A Handbook of Lattice Spacings and Structures of Metals and Alloys," Pergamon Press, New York, 1958-1967.
8. Barrett, C. S.: "Structure of Metals," 3d ed., McGraw-Hill Book Company, New York, 1966.
9. Lipson, H., and C. A. Taylor: "Fourier Transforms and X-ray Diffraction," G. Bell & Sons, Ltd., London, 1958.

9a-2. Effect of Symmetries on Tensor Properties for Crystals.¹ The point-group symmetries inherent in the 32 crystal classes have an effect on the types of relations that can exist between electric, magnetic, thermal, optical, and elastic stress variables and their corresponding strain variables. Such relations are usually expressed in tensor form and for cartesian coordinates can be expressed in terms of simple cartesian tensors. With such tensors, the transformations considered are restricted to be orthogonal transformations from one cartesian system to another. By this restriction, we are avoiding many complications which arise in the case of oblique coordinates or nonplanar coordinate surfaces.

The simplest relations exist between scalar quantities and *first-rank tensors* (vectors). Examples are given by the pyroelectric effect, the electrocaloric effect, the heat of polarization, and the field due to increase in thermal energy, which satisfy the equations

$$D_n = p_n \Delta T \quad \Delta S = p_i E_i \quad \Delta S = q_n D_n \quad E_i = -q_i \Delta T \quad (9a-1)$$

where the symbols and their meaning are given in Table 9a-8. First-rank tensors can also arise from a contracted third-rank tensor. An example of interest is the piezoelectric displacement due to a hydrostatic pressure:

$$D_n = d_{nkk} T_{kk} \quad (9a-2)$$

Table 9a-4 shows the resulting constants for the various crystallographic symmetries. Only those classes which have unique polar axes have constants different from zero.

TABLE 9a-4. FIRST-RANK TENSORS

| | |
|-------------------------------------|---|
| 1; q_1, q_2, q_3 | 2; 0, $q_2, 0$ ($y = \text{unique axis}$) |
| m ; $q_1, 0, q_3$ ($m \perp y$) | $mm2, 4, 4mm, 3, 3m, 6, 6mm; 0, 0, q_3$ |

All other classes have a zero result. All classes giving a positive result have a unique polar axis.

Second-rank tensors can arise as a relation between two vectors or as a relation between a scalar and a quantity expressed by a second-rank tensor. Examples of the first case are electric permittivity, dielectric impermeability, magnetic permeability and magnetic impermeability, electric conductivity and resistivity, thermal conductivity and resistivity, and Thomson thermoelectricity (ref. 2). Equations for these effects are given by (9a-3) with a glossary of terms in Table 9a-8:

$$\begin{aligned} D_i &= \epsilon_{ij} E_j & E_i &= \beta_{ij} D_j & B_i &= \mu_{ij} H_j \\ H_i &= \beta_{ij} B_j & I_i &= \sigma_{ij} E_j & E_i &= \rho_{ij} I_j \\ h_i &= -k_{ij} \left(\frac{\partial T}{\partial x_j} \right) & \frac{\partial T}{\partial x_i} &= -r_{ij} h_j & \frac{\partial \bar{\mu}}{\partial x_i} &= -\sum_{ik} \frac{\partial T}{\partial x_k} \end{aligned} \quad (9a-3)$$

Examples of the second case for which the tensors arise as a relation between a scalar and quantities expressed as second-rank tensors are thermal expansions, stresses due to temperature changes, strain for a hydrostatic stress, and Peltier thermoelectric coefficients. These relations are given by Eq. (9a-4):

$$S_{ij} = \alpha_{ij} \Delta T \quad T_{ij} = -\lambda_{ij} \Delta T \quad S_{ij} = s_{ijkl} T_{kk} \quad \Pi_{ik} = \frac{T}{e} \Sigma_{ik} \quad (9a-4)$$

All the second-rank tensors are symmetric except the thermoelectric tensors. Table 9a-5 shows the terms for the various crystal symmetries and the changes caused by the relations $\alpha_{ij} = \alpha_{ji}$.

¹This subsection was originally contributed by W. P. Mason and E. A. Wood, Bell Telephone Laboratories, Inc.

Third-rank tensors have been employed in expressing the direct and inverse piezo-electric effect with four different forms depending on the sets of variable used. They have also been employed in defining the electrooptical effect and the Hall effect. These relations are given by Eq. (9a-5):

$$\begin{aligned} D_n &= d_{nij}T_{ij} & S_{ij} &= d_{mij}E_m & T_{kl} &= -e_{mkl}E_m & D_n &= e_{nij}S_{ij} \\ T_{kl} &= -h_{nkl}D_n & E_m &= -h_{mij}S_{ij} & S_{ij} &= g_{nij}D_n & E_m &= -g_{mij}T_{ij} \\ E_m &= D_n(\beta_{mn}^S + \gamma_{mno}^S D_o) & E_i &= \epsilon_{ijk}I_j(R_{km}H_m) \end{aligned} \quad (9a-5)$$

In all third-rank tensors two pairs of indices can be interchanged, for example ij in

TABLE 9a-5. SECOND-RANK TENSORS

| | | |
|---|--|--|
| Triclinic 1, $\bar{1}$ 9 constants | π_{11} π_{12} π_{13} π_{21} π_{22} π_{23} π_{31} π_{32} π_{33} | If symmetric $\alpha_{12} = \alpha_{21}$; $\alpha_{13} = \alpha_{31}$ $\alpha_{23} = \alpha_{32}$; 6 constants |
| Monoclinic 2, m , $2/m$ 5 constants | π_{11} 0 π_{13} 0 π_{22} 0 π_{31} 0 π_{33} | If symmetric $\alpha_{13} = \alpha_{31}$ 4 constants |
| Trigonal, tetragonal, hexagonal 3, $\bar{3}$, 4, $\bar{4}$, $4/m$ 6, $\bar{6}$, $6/m$ 3 constants | π_{11} π_{12} 0 $-\pi_{12}$ π_{11} 0 0 0 π_{33} | If symmetric $\alpha_{12} = 0$ 2 constants |
| Trigonal, tetragonal, hexagonal 32, $3m$, $\bar{3}m$ 422, $4mm$, $\bar{4}2m$, $4/mmm$ 622, $6mm$, $\bar{6}m2$, $6/mmm$ 2 constants | π_{11} 0 0 0 π_{11} 0 0 0 π_{33} | If symmetric the same number of constants |
| Cubic or isotropic 23, $m\bar{3}$, $\bar{4}3m$ 432, $m3m$ 1 constant | π_{11} 0 0 0 π_{11} 0 0 0 π_{11} | Same for symmetric tensor |

d_{nij} , since T_{ij} is a symmetric tensor with $T_{ij} = T_{ji}$. Hence it is usual to replace the two indices by a single one according to the convention

$$11 = 1 \quad 22 = 2 \quad 33 = 3 \quad 23 = 32 = 4 \quad 13 = 31 = 5 \quad 12 = 21 = 6 \quad (9a-6)$$

Table 9a-6 gives the resulting third-rank tensors for the various crystal symmetries.

All the *fourth-rank tensors* in general use express relations between two second-rank tensors such as stress and strain or between a second-rank tensor and the product of two vectors. Examples are elasticity equations, photoelastic relations, magnetostrictive and electrostrictive relations, magnetoresistance effects, and piezoresistance effects, expressed by the equations

$$\begin{aligned} S_{ij} &= s_{ijk}T_{kl} & T_{kl} &= c_{ijkl}S_{ij} & E_m &= D_n(\beta_{mn}^S + m_{ijmn}S_{ij}) \\ S_{ij} &= M_{ijk}B_kB_l & S_{ij} &= q_{ijkl}D_kD_l & E_i &= \alpha_{ijk}I_jH_kH_l \\ E_i &= (\rho_{ij} + \pi_{ijk}T_{kl})I_j \end{aligned} \quad (9a-7)$$

Except in the case of ferroelectric or ferromagnetic crystals (ref. 13), it is generally believed that $T_{ij} = T_{ji}$, so that the compliance tensor s_{ijk} and the elastic stiffness tensor c_{ijkl} would indicate 36 independent constants. On account of Maxwell-type

TABLE 9a-6. THIRD-RANK TENSORS

| | e_{11} | e_{12} | e_{13} | e_{14} | e_{15} | e_{16} | e_{21} | e_{22} | e_{23} | e_{24} | e_{25} | e_{26} | e_{31} | e_{32} | e_{33} | e_{34} | e_{35} | e_{36} | |
|-------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|---|
| 1 | e_{11} | e_{12} | e_{13} | e_{14} | e_{15} | e_{16} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| | e_{21} | e_{22} | e_{23} | e_{24} | e_{25} | e_{26} | e_{21} | e_{22} | e_{23} | e_{24} | e_{25} | e_{26} | e_{31} | e_{32} | e_{33} | e_{34} | e_{35} | e_{36} | |
| | e_{31} | e_{32} | e_{33} | e_{34} | e_{35} | e_{36} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| $\bar{1}$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| m | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | e_{11} | e_{12} | e_{13} | e_{14} | e_{15} | e_{16} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| $mm2$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | e_{11} | e_{12} | e_{13} | e_{14} | e_{15} | e_{16} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| $4, 6$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | e_{11} | e_{12} | e_{13} | e_{14} | e_{15} | e_{16} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 422 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 622 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | e_{11} | e_{12} | e_{13} | e_{14} | e_{15} | e_{16} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 422 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 622 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | e_{11} | e_{12} | e_{13} | e_{14} | e_{15} | e_{16} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 3 | e_{11} | e_{12} | e_{13} | e_{14} | e_{15} | e_{16} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | e_{21} | e_{22} | e_{23} | e_{24} | e_{25} | e_{26} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | e_{31} | e_{32} | e_{33} | e_{34} | e_{35} | e_{36} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| $\bar{6}$ | e_{11} | e_{12} | e_{13} | e_{14} | e_{15} | e_{16} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | e_{21} | e_{22} | e_{23} | e_{24} | e_{25} | e_{26} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | e_{31} | e_{32} | e_{33} | e_{34} | e_{35} | e_{36} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| $\bar{6}m2$ | e_{11} | e_{12} | e_{13} | e_{14} | e_{15} | e_{16} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | e_{21} | e_{22} | e_{23} | e_{24} | e_{25} | e_{26} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | e_{31} | e_{32} | e_{33} | e_{34} | e_{35} | e_{36} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |

For all systems with a center of symmetry, the third rank tensors vanish.

4/mmm = 0

3 = 0

3m = 0

6/mmm, 6/m
m3, m3m, 432 = 0

TABLE 9a-7. FOURTH-RANK TENSORS

| | (Type $M_{ijkl}, i \rightarrow j, k \rightarrow l$; $M_{11}, M_{12}, M_{13}, M_{21}, M_{22}, M_{23}, M_{31}, M_{32}, M_{33}$) | (Type $c_{ij}, i \rightarrow j, k \rightarrow l, \psi \rightarrow k, l$; $M_{15}, M_{25}, M_{35}, M_{45}, M_{55}, M_{65}$) | (Type $K_{ijkl}, i \rightarrow j \rightarrow k \rightarrow l$; $M_{16}, M_{26}, M_{36}, M_{46}, M_{56}, M_{66}$) | |
|--|--|---|---|--|
| Group I Triclinic $1, \bar{1}$ 36 constants | $M_{11}, M_{12}, M_{13}, M_{21}, M_{22}, M_{23}, M_{31}, M_{32}, M_{33}, M_{41}, M_{42}, M_{43}, M_{51}, M_{52}, M_{53}, M_{61}, M_{62}, M_{63}$ | $M_{15}, M_{25}, M_{35}, M_{45}, M_{55}, M_{65}$ | $M_{16}, M_{26}, M_{36}, M_{46}, M_{56}, M_{66}$ | c constants the same except $c_{66} = c_{60}$, resulting in 21 constants. K constants the same as c except $K_{44} = K_{23}, K_{55} = K_{13}, K_{66} = K_{12}, K_{46} = K_{25}, K_{56} = K_{14}, K_{45} = K_{36}$, resulting in 15 constants. |
| Group II Monoclinic $2, m, 2/m$ 20 constants $y =$ unique axis | $M_{11}, M_{12}, M_{22}, M_{31}, M_{32}, M_{33}, M_{41}, M_{42}, M_{43}, M_{51}, M_{52}, M_{53}, M_{61}, M_{62}, M_{63}$ | $M_{15}, M_{25}, M_{35}, M_{45}, M_{55}, M_{65}$ | $M_{16}, M_{26}, M_{36}, M_{46}, M_{56}, M_{66}$ | c constants the same except $c_{46} = c_{60}$, resulting in 13 constants. K constants the same as c , except $K_{44} = K_{23}, K_{55} = K_{13}, K_{66} = K_{12}, K_{46} = K_{25}$, resulting in 9 constants. |
| Group III Orthorhombic $mm2, 222, mmm$ 12 constants | $M_{11}, M_{12}, M_{13}, M_{21}, M_{22}, M_{23}, M_{31}, M_{32}, M_{33}, M_{41}, M_{42}, M_{43}, M_{51}, M_{52}, M_{53}, M_{61}, M_{62}, M_{63}$ | $M_{15}, M_{25}, M_{35}, M_{45}, M_{55}, M_{65}$ | $M_{16}, M_{26}, M_{36}, M_{46}, M_{56}, M_{66}$ | c constants the same except $c_{36} = c_{60}$, resulting in 9 constants. K constants the same as c except $K_{44} = K_{23}, K_{55} = K_{13}, K_{66} = K_{12}$, resulting in 6 constants. |
| Group IV Trigonal $3, \bar{3}$ 12 constants | $M_{11}, M_{12}, M_{13}, M_{21}, M_{22}, M_{23}, M_{31}, M_{32}, M_{33}, M_{41}, M_{42}, M_{43}, M_{51}, M_{52}, M_{53}, M_{61}, M_{62}, M_{63}$ | $M_{15}, M_{25}, M_{35}, M_{45}, M_{55}, M_{65}$ | $M_{16}, M_{26}, M_{36}, M_{46}, M_{56}, M_{66}$ | c constants the same, except $c_{ab} = c_{10}$ and $c_{82} = c_{46} = 0$. $c_{46} = c_{25}, c_{56} = c_{14}$, resulting in 7 constants. K constants the same as c constants except $K_{44} = K_{23}$, resulting in 6 constants. |
| Group V Trigonal $3m, 32, \bar{3}m$ 8 constants | $M_{11}, M_{12}, M_{13}, M_{21}, M_{22}, M_{23}, M_{31}, M_{32}, M_{33}, M_{41}, M_{42}, M_{43}, M_{51}, M_{52}, M_{53}, M_{61}, M_{62}, M_{63}$ | $M_{15}, M_{25}, M_{35}, M_{45}, M_{55}, M_{65}$ | $M_{16}, M_{26}, M_{36}, M_{46}, M_{56}, M_{66}$ | c constants the same except $c_{ab} = c_{60}, 2c_{41} = c_{14} = c_{56}$. 6 constants. K constants the same as the c constants except $K_{44} = K_{23}$. 5 constants. |
| Group VI Tetragonal $4, 4, 4/m$ 10 constants | $M_{11}, M_{12}, M_{13}, M_{21}, M_{22}, M_{23}, M_{31}, M_{32}, M_{33}, M_{41}, M_{42}, M_{43}, M_{51}, M_{52}, M_{53}, M_{61}, M_{62}, M_{63}$ | $M_{15}, M_{25}, M_{35}, M_{45}, M_{55}, M_{65}$ | $M_{16}, M_{26}, M_{36}, M_{46}, M_{56}, M_{66}$ | c constants the same except $c_{13} = c_{31}, c_{16} = c_{61}, c_{45} = 0$. 7 constants. K constants the same except $K_{44} = K_{23}, K_{16} = K_{15}$. 5 constants. |

TABLE 9a-7. FOURTH-RANK TENSORS (Continued)

| Group | Crystal System | M_{11} | M_{12} | M_{13} | M_{22} | M_{23} | M_{33} | M_{44} | M_{55} | M_{66} | Constants |
|--|----------------|----------|----------|----------|-------------------|----------|----------|----------|----------|-------------------|--|
| Group VII Tetragonal $4mm, 42m, 422, 4/mmm$ 7 constants | | M_{11} | M_{12} | M_{13} | 0 | 0 | 0 | 0 | 0 | 0 | c constants the same except $c_{13} = c_{31}$. 6 constants. |
| | | M_{12} | M_{11} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | K constants the same except $K_{44} = K_{33}, K_{16} = K_{15}$. 4 constants. |
| | | 0 | 0 | 0 | M_{44} | 0 | 0 | 0 | 0 | M_{66} | |
| Group VIII Hexagonal $6, 6, 6/m$ 8 constants | | M_{11} | M_{12} | M_{13} | 0 | 0 | 0 | 0 | 0 | 0 | c constants the same except $c_{13} = c_{31}, c_{61} = 0, c_{45} = 0$. 5 constants. |
| | | M_{12} | M_{11} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | K constants the same as c constants except $K_{44} = K_{23}$. 4 constants. |
| | | M_{31} | 0 | 0 | M_{44} | M_{45} | 0 | 0 | 0 | 0 | |
| | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | $M_{11} - M_{12}$ | |
| Group IX Hexagonal $6m2, 622, 6mm, 6/mmm$ 6 constants | | M_{11} | M_{12} | M_{13} | 0 | 0 | 0 | 0 | 0 | 0 | c constants the same except $c_{13} = c_{31}$. 5 constants. |
| | | M_{12} | M_{11} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | K constants the same as c constants, except $K_{44} = K_{23}$. 4 constants. |
| | | M_{31} | 0 | 0 | M_{44} | 0 | 0 | 0 | 0 | 0 | |
| | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | $M_{11} - M_{12}$ | |
| Group X Cubic $23, m3$ 4 constants | | M_{11} | M_{12} | M_{13} | 0 | 0 | 0 | 0 | 0 | 0 | c constants the same except $c_{12} = c_{13}$. 3 constants. |
| | | M_{12} | M_{11} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | K constants the same as c constants except $K_{44} = K_{12}$. 2 constants. |
| | | 0 | 0 | 0 | M_{44} | 0 | 0 | 0 | 0 | 0 | |
| | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | M_{44} | |
| Group XI Cubic $43m, 432, m3m$ 3 constants | | M_{11} | M_{12} | M_{13} | 0 | 0 | 0 | 0 | 0 | 0 | c constants the same. 3 constants. |
| | | M_{12} | M_{11} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | K constants the same as c constants except $K_{44} = K_{12}$. 2 constants. |
| | | 0 | 0 | 0 | M_{44} | 0 | 0 | 0 | 0 | 0 | |
| | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | M_{44} | |
| Group XII Isotropic 2 constants | | M_{11} | M_{12} | M_{13} | 0 | 0 | 0 | 0 | 0 | 0 | c and K constants the same. 2 constants. |
| | | M_{12} | M_{11} | 0 | 0 | 0 | 0 | 0 | 0 | 0 | |
| | | 0 | 0 | 0 | $M_{11} - M_{12}$ | 0 | 0 | 0 | 0 | 0 | |
| | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | $M_{11} - M_{12}$ | |

relations, one can interchange the ij with the kl moduli, and this reduces the number to 21. When it is not permissible to interchange ij with kl as in the magnetostrictive equations,

$$S_{ij} = M_{ijkl} B_k B_l \quad (9a-8)$$

there are 36 possible constants. Table 9a-7 for fourth-rank tensors shows how the crystal symmetries affect the number and relations among the independent constants. Type c relations indicated are for the case that ij can be interchanged with kl . A

TABLE 9a-8. GLOSSARY OF TENSOR TERMS

| <i>Symbol</i> | <i>Meaning</i> | <i>Symbol</i> | <i>Meaning</i> |
|---------------|--|------------------|---|
| ΔQ | Increment of heat | r_{ij} | Thermal resistive constants |
| ΔT | Increment of temperature | R_{kl} | Hall-effect constants |
| ΔS | Increment of entropy | s_{ijkl} | Compliance constants |
| B_i | Magnetic flux density | S_{ij} | Strain components |
| c_{ijkl} | Elastic stiffness constants | T | Absolute temperature |
| D | Electric displacements | T_{kl} | Stress components |
| D_o | Electric displacement at optical frequencies | x_i | Length variable |
| d_{nij} | Piezoelectric constants | α_{ij} | Temperature-expansion coefficients |
| e | Electronic charge | α_{ijkl} | Magnetostrictive constants |
| e_{mkl} | Piezoelectric constants | β_{ij} | Dielectric or magnetic impermeabilities |
| E | Electric fields | ν_{mno} | Electrooptic constants |
| g_{nij} | Piezoelectric constants | ϵ_{ij} | Dielectric constants |
| h_i | Flow of heat per unit area | ϵ_{ijk} | Rotation tensor (see ref. 4, p. 393) |
| h_{nkl} | Piezoelectric constants | λ_{ij} | Temperature coefficients of stress at constant volume |
| H_j | Magnetic fields | $\bar{\mu}$ | Electrochemical potential |
| I_i | Electric current densities | μ_{ij} | Magnetic permeability constants |
| k_{ij} | Thermal conductivities | π_{ijkl} | Piezoresistive constants |
| m_{ijmn} | Photoelastic constants | Π_{ik} | Peltier thermoelectric coefficients |
| M_{ijkl} | Magnetostrictive constants | ρ_{ij} | Electrical resistivity constants |
| p_n, p_i | Pyroelectric or pyromagnetic constants | σ_{ij} | Electrical conductivity constants |
| P_i | Polarization | Σ_{ik} | Thermoelectric coefficients (Thomson) |
| q_n, q_i | Pyroelectric or pyromagnetic constants | | |
| q_{ijkl} | Electrostrictive constants | | |

third type of symmetry for fourth-rank tensors occurs when all the indices $i, j, k,$ and l are interchangeable. Such a case occurs when the elastic moduli satisfy the Cauchy relationship. This is denoted by type- K symmetry in Table 9a-7.

Table 9a-8 shows the symbols used in the above equations and their meaning.

References for Section 9a-2

1. Mason, W. P.: "Piezoelectric Crystals and Their Application to Ultrasonics," D. Van Nostrand Company, Inc., Princeton, N.J., 1940.
2. Nye, J. F.: "Physical Properties of Crystals," Oxford University Press, New York, 1957.
3. Huntington, H. B.: The Elastic Constants of Crystals, *Solid State Phys.* **7** (1958).
4. Mason, W. P.: "Physical Acoustics and the Properties of Solids," D. Van Nostrand Company, Inc., Princeton, N.J. 1958.